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SUBJECT: Authorization for Release of Technical Information, Control Number: AFRL-PR-ED-TP-2002-106
J. Mike Fife (PRSS) *et al.*, "Initial Use of a 3-D Plasma Simulation System for Predicting Surface
Sputtering and Contamination by Hall Thrusters"

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(Statement A)

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PHILIP A. KESSEL

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Technical Advisor

Space and Missile Propulsion Division

Initial Use of a 3-D Plasma Simulation System for Predicting Surface Sputtering and Contamination by Hall Thrusters

J. M. Fife and M. R. Gibbons
U.S. Air Force Research Laboratory
Edwards AFB, CA

D. B. VanGilder and D. E. Kirtley
ERC, Inc.
Edwards AFB, CA

A 3-D Plasma Interaction Modeling System is being developed to predict the interaction of electric propulsion plumes with surfaces. The system, named COLISEUM, is designed to be flexible, usable, and expandable, allowing users to define surfaces with their choice of off-the-shelf 3-D solid modeling packages. These surfaces are then loaded into COLISEUM, which performs plasma operations based on user commands. Functional modules are interchangeable, and can range from simple (prescribed plume field) to complex (PIC-DSMC). Surface interaction parameters such as ion flux, ion energy, sputtering, and re-deposition are computed. Development to date has progressed to include the two simplest functional modules: *prescribed plume*, which imports and superimposes a plume distribution, and *ray*, which performs ray tracing of flux from point sources. More sophisticated functional plasma simulation modules such as PIC-Hybrid-MCC are currently being integrated. This paper presents some of the first COLISEUM results -- sputtering and re-deposition predictions on a spacecraft and in a vacuum chamber due to operation of Hall-effect thrusters.

Introduction

Onboard electric propulsion (EP) thrusters, which use electric power to generate or augment thrust, hold the promise of greatly increased satellite maneuverability, and enabling new missions. Many types of EP thrusters are already in mature states of development, and many can achieve specific impulses over 3000 seconds. This, combined with growing electric power levels onboard new-generation spacecraft, is pushing EP rapidly into the mainstream.^{1,2}

Several EP devices are currently being evaluated for use onboard U.S. commercial and military spacecraft. One of the most promising for near-term use is the Hall-effect thruster (HET). Over 120 HETs have flown on Russian spacecraft, where typical flight units have specific impulses around 1600 seconds and efficiencies near 50%.³ HETs operate by generating a stationary xenon plasma inside an annular channel. Strong radial magnetic fields are applied which impede electron motion, but allow ions to accelerate axially out of the device with velocities around 20 km/s (energies of around 300 eV).

High-energy HET exhaust ions may erode (sputter) surfaces on which they impinge. In addition, this sputtered material may be re-deposited on other spacecraft surfaces. These issues, and others, such as electromagnetic interference and spacecraft charging, cause some concern for spacecraft designers who want the maneuverability EP offers but do not want increased risk.

Efforts are underway to quantify some of the risks associated with integration of EP with spacecraft, including surface erosion and re-deposition. Work has been done to computationally model expansion of HET plumes.⁴ Additionally, Gardner et al. have developed Environment Work Bench (EWB), a code that calculates sputtering of spacecraft surfaces by superimposing pre-computed EP plumes onto spacecraft geometries.⁵ However, existing codes do not self-consistently calculate the plume expansion with the 3-D surface geometry in a usable, flexible way.

The Air Force Research Laboratory is leading development of a new software package named COLISEUM, which is capable of self-consistently modeling plasma propagation and interactions with arbitrary 3-D surfaces. Three important requirements have been placed on COLISEUM: It must be **USABLE**, **FLEXIBLE**, and **EXPANDABLE**.

USABLE means a typical engineer should be able to set up and run a typical low-fidelity case in less than one day with less than three days training.

FLEXIBLE means COLISEUM must be able to simulate at least three important cases: a) a single spacecraft, b) multiple spacecraft in formation, and c) laboratory conditions (e.g. the interior of a vacuum test facility). Simulating laboratory conditions is very important for two reasons. First, since there is very little on-orbit data for EP thrusters, ground-based tests must be relied upon for the bulk of code validation. Second, by modeling the laboratory conditions, COLISEUM can help engineers interpret lab measurements.

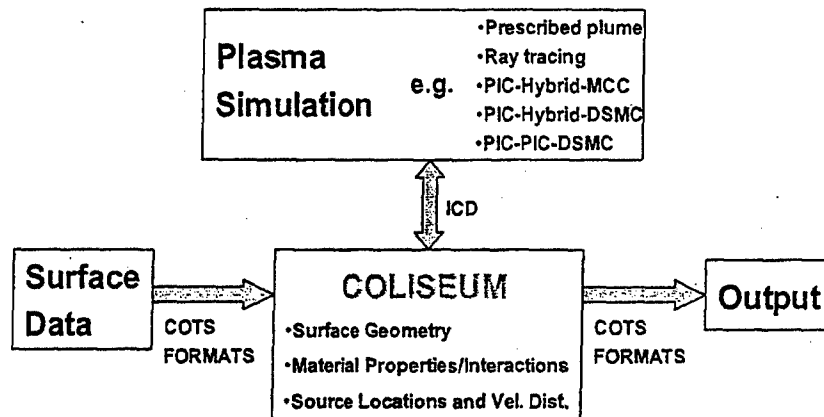


Fig. 1 Architecture for using various interchangeable plasma simulation techniques with the same 3-D surface geometry.

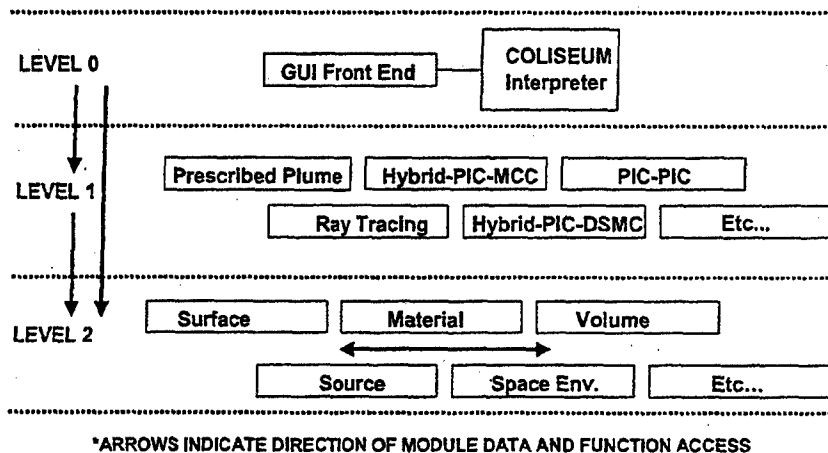


Fig. 2 COLISEUM data structure. Each module represents a cohesive block of code and data with a specific function.

In addition to being able to simulate multiple geometries, COLISEUM must be flexible in its use of plasma simulation algorithms. It must be able to use a variety of interchangeable plasma simulation algorithms for each geometry. Therefore, if low run-time is desired, a low-fidelity technique can be selected such as ray tracing. For higher fidelity (at the cost of longer run-time), something like Particle-In-Cell (PIC) can be used.

EXPANDABLE means COLISEUM can be easily expanded to incorporate new plasma simulation algorithms, new capabilities, or improved efficiency. Furthermore, as new plasma simulation algorithms are added, old ones must continue to work.

Approach

Fig. 1 shows how COLISEUM integrates surface geometries with a suite of various interchangeable plasma simulations. In general, COLISEUM can be viewed as a toolbox or

framework in which 3-D plasma simulations can be quickly integrated. Common calculations (such as those related to surfaces, material properties, and flux sources) are standardized and provided as resources (data and subroutines) to each simulation.

From a code architecture standpoint, COLISEUM has been designed as a collection of modules, each with a specific function and hierarchy. Each module contains data and associated code. Modules may be categorized into three levels, as shown in Fig. 2.

Level 0 modules perform functions related to user-interaction. Although COLISEUM is fundamentally command-driven, a Graphical User Interface (GUI) front end is envisioned for the future.

Level 1 modules are the primary components of COLISEUM. They calculate plasma propagation on the volume domain. They contain algorithms, such as fluid, PIC, DSMC, or

Table 1 Sputter yield coefficients for bombardment by singly ionized xenon

Material	Coefficient a	Coefficient b (J^{-1})
Al	1.0	1.9e16
ITO	0.1	6.25e15
Kapton	0.05	2.5e14
AgT5	1.0	1.9e16

hybrids thereof, which perform a solution subject to pre-set boundary conditions. Level 1 modules are uniform and interchangeable. They all conform to a specific Interface Control Document (ICD) – they have specific inputs, outputs, and resources available to them.

Level 2 modules perform support tasks common to all types of plasma simulations. They handle boundary conditions, and provide support to Level 1 modules. They act as a toolbox or collection of resources.

The purpose of the modular design is to give COLISEUM flexibility and expandability. A large number of Level 1 modules are desired to allow flexibility in solving a variety of different problems. The ICD is, therefore, very important, because it describes for authors of Level 1 modules a) what inputs and boundary conditions must be recognized, b) what outputs are expected, and c) what Level 2 resources are available. The ICD may be distributed to outside groups so that COLISEUM can be expanded through addition of new Level 1 modules.

Surfaces

Surfaces are modeled in finite-element fashion as contiguous triangular elements joined at the vertices (nodes). COLISEUM does not generate 3-D geometries or surfaces; instead, it imports them from other software.

Users create custom geometries using almost any mainstream commercial 3-D solid modeling package. Then, they use finite element analysis software to mesh the surface of their geometry as if they were going to perform a structural analysis using thin shells. The user then saves the meshed surface file in ANSYS format, which is readable by COLISEUM. ANSYS finite element format was chosen because it is widely supported by finite element packages.

This concept of separating the surface geometry definition from the plasma calculation has proven very successful. It greatly reduced development time and cost by eliminating the need for a separate surface definition module. It allows users to choose which software to use in defining geometries. And, users can import into COLISEUM geometries that have already been defined for other reasons (structural, thermal, etc.).

Material Properties

The user constructs a database of materials that is read by COLISEUM. The database contains material names, material reference numbers, and molecular weights and charges (in the case of ions). Materials in the database are connected to the

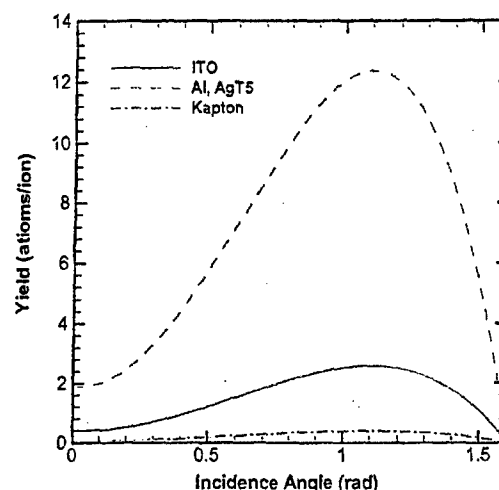


Fig. 3. Sputter yields for bombardment by singly ionized xenon at 300eV.

surface geometry by the material reference number. Users mark surface materials during geometry/surface definition using their finite element software. They simply set the elastic modulus of the surface component to be equal to the material reference number. This value appears in the ANSYS file, where COLISEUM reads it.

The user also provides a second database, a materials interaction database. This database contains the sputter yield coefficients and sticking coefficients of one material interacting with the other. For example, one important interaction may be between Xe^+ and Kapton.

The material interaction database can support multiple surface sputtering models. Currently, a model by Gardner et al.⁶ is implemented for generating the sputter yield for each species as a function of the ion energy and incidence angle:

$$Y(E, \theta) = (a + bE)(1.0 - 0.72\theta + 11.72\theta^2 - 3.13\theta^3 - 2.57\theta^4)$$

Above, E is the particle energy, and θ is the incidence angle (off-normal). Table 1 gives the coefficients for the materials used here, indium titanium oxide (ITO), aluminum, silver with Teflon coating, Kapton. ITO is commonly used as an anti-reflective coating on solar array cover glass. Fig. 3 plots sputter yield for $E=300\text{eV}$.

Redeposition is currently calculated by ray tracing. The sputtered flux is distributed as the cosine of the off-normal angle and projected from the sputtering elements to all other viewable surface elements. This simple model will be replaced by more detailed models in the future.

Sources

Sources are modeled as having a specific velocity distribution that is constant over individual surface elements. A collection of Level 2 commands allows the user to either specify one of a set of source types (mono-energetic, half-Maxwellian, etc.)

or read in a file containing a custom discretized velocity distribution function.

Source elements are identified with a source reference number during geometry/surface definitions, much like the materials are identified.

This method is extremely descriptive and general. Level 1 modules may treat this information in various ways. For instance, a Level 1 module could be written to treat the source element a single point source for ray tracing purposes. Alternately, particle methods could sample from the velocity distribution and introduce particles randomly over the full element surface. Therefore, this choice of source definition methods gives COLISEUM great flexibility.

Plasma Simulation

Currently, two Level 1 modules have been written. The first, **PRESCRIBED_PLUME**, allows the user to import a previously calculated or measured plume field. This plume is superimposed over the user's surface geometry. Plasma densities, fluxes, and sputter rates are then calculated at each surface node.

The second module, **RAY**, uses ray tracing to calculate the flux from all sources onto all surface nodes. Once again, density, flux, and sputter rate are calculated.

Future modules will incorporate statistical kinetic methods for plasma calculation such as PIC and DSMC. Plans also include development of kinetic algorithms for use on unstructured meshes, adaptive meshes, and domain decomposition. Primarily, these techniques will be incorporated to add flexibility to the simulation. For instance, domain decomposition will allow the domain to be broken into smaller sub-domains, each potentially having different algorithms, depending on local parameters as the Debye length or mean free path.

```
# coliseum.in
#
# Load a GEO satellite geometry,
# add a 3kW HET source, calculate
# the flux and sputtering using
# ray tracing, and save the
# results in Tecplot format.
#

material_load material.txt mat_mat.txt

surface_load ANSYS GEO_Sat.ANS

source_specify 18 FLUX_PHI 0007 het_3kw.dat
12e-6 16000.0 1.0

ray DEPOSIT

surface_save TECPLOT GEO_Sat.dat
FLUXNORMAL0007 SPUTERRATE
```

Fig. 4 Sample COLISEUM command file

User Interface

The user enters commands via a COLISEUM input file. The commands are executed sequentially as they appear in the input file. Each command may have some number of parameters separated by spaces or commas. A sample input file is shown in Fig. 4.

Typical run times for low-fidelity cases (using **PRESCRIBED_PLUME** or **RAY**) take approximately 20 seconds on a 2 GHz Intel Pentium 4 workstation. Once more detailed physics are incorporated, with Level 1 modules incorporating such algorithms as PIC-DSMC, run times are expected to be between 20 minutes and 20 hours, depending on the level of fidelity and on the initial conditions.

Results and Discussion

In initial tests, COLISEUM, runs were executed for two cases: a) a fictitious geosynchronous satellite with an HET firing in the north direction (as if for stationkeeping), and b) an HET firing inside a vacuum chamber (as if during a flight readiness test). In both cases, the Level 1 module, **PRESCRIBED_PLUME** was used to incorporate a previously calculated plume expansion model onto the surface geometry. The plume expansion model used here was calculated for a Busek 200-Watt HET⁷ by SAIC using the GILBERT⁵ toolbox.

Results from the first case are shown in Fig. 5 through Fig. 8. Fig. 5 shows the geometry of the geosynchronous satellite model, with surfaces broken down into triangular elements. Two commercial packages, SolidWorks and COSMOS/DesignStar, were used to generate these surface geometries. Final plotting was performed by another commercially available package, Tecplot. The colors of the mesh lines indicate the type of material. Fig. 6 shows a slice through the 200-Watt HET plume superimposed on the satellite model. Plasma density is highest near the HET exhaust, and drops off rapidly as the plume expands upward toward the solar arrays. Fig. 7 shows the COLISEUM calculation of surface sputtering rate. Finally, the rate of redeposition of ITO from the solar array coverglass is shown in Fig. 8.

The sputtering rate peaks near the solar array corner. This illustrates a real problem with electric propulsion on geosynchronous satellites. For north-south stationkeeping, the ideal firing direction (from a thrust efficiency standpoint) is directly north. However, COLISEUM shows us that long-term firing of the HET over the lifetime of a satellite (~7000 hours) in this configuration may remove 2.5 mm from the surface of the solar array at the corner. In reality, the solar array will be rotating to track the sun, and will not always have a corner directly in the HET plume. So 2.5 mm can be considered a worst case. Other ways of reducing the sputtering are to angle the HET plume away from due north.

Results from the second case are shown in Fig. 9 through Fig. 12. Fig. 9 shows the geometry of the interior of a vacuum chamber, with an HET in the center, and several plasma diagnostic instruments arrayed nearby. Once again the 200-Watt HET plume is incorporated, and fluxes, sputtering rates, and redeposition rates are calculated by COLISEUM.

Referring to Fig. 11, a spherical plasma probe can be seen protruding from the instrumentation panel. Maximum ion flux to this probe is approximately $1 \times 10^{18} \text{ m}^{-2} \text{ s}^{-1}$ at the point nearest the HET. However, maximum sputter rate appears as a ring around the point on the probe nearest the HET. This is due to the dependency of sputter yield on incidence angle. Sputter rate at normal incidence is typically lower than that at grazing angles, as can be seen in the discussion of sputter models above.

The redeposition rate of aluminum from the chamber wall can be seen in Fig. 12. It shows that significant amounts of aluminum re-deposit onto the HET and other instrumentation inside the chamber. This metal redeposition from the chamber walls has been observed in numerous tests at AFRL.

Currently, COLISEUM calculates sputter rate and redeposition rate independently. Therefore, NET sputter or NET deposition rate must be inferred from the independent calculations. The places where sputter rate is higher than redeposition rate are expected to exhibit sputter-cleaning, i.e. no net redeposition. Places where redeposition exceeds sputter rate are expected to exhibit net deposition. Later versions of COLISEUM will iteratively converge on a NET sputter or NET deposition rate for each surface element, at which time comparisons may be made with experimental measurements.

Conclusions

Although still in an early stage of development, COLISEUM now can help predict ion flux and sputtering of surface materials both onboard spacecraft and in laboratory test facilities. COLISEUM's modular architecture is allowing rapid expansion of its capabilities, and giving users flexibility to design their own geometries and choose their preferential plasma simulation method.

Additional work for the future includes expansion of the source module, incorporation of surface re-deposition, and construction of new Level 1 modules that can self-consistently compute plasma expansion and interaction with surfaces.

References

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- ⁷V. Hruby, J. Monheiser, B. Pote, C. Freeman, and W. Connolly, "Low Power, Hall Thruster Propulsion System," IEPC-99-092, 26th International Electric Propulsion Conference, 17-21 October, 1999, Kitakyushu, Japan.

CASE 1 – Geosynchronous Satellite with HET for North-South Stationkeeping

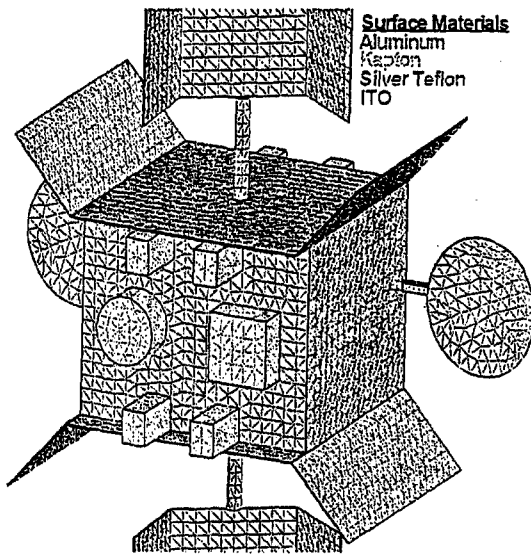


Fig. 5. Surface mesh of a geosynchronous satellite geometry with eight HETs positioned for north-south stationkeeping.

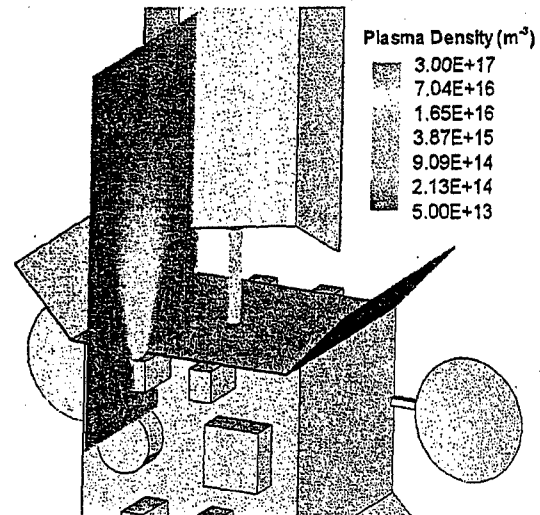


Fig. 6. Slice showing plasma density from a 200-Watt HET firing onboard a geosynchronous satellite.

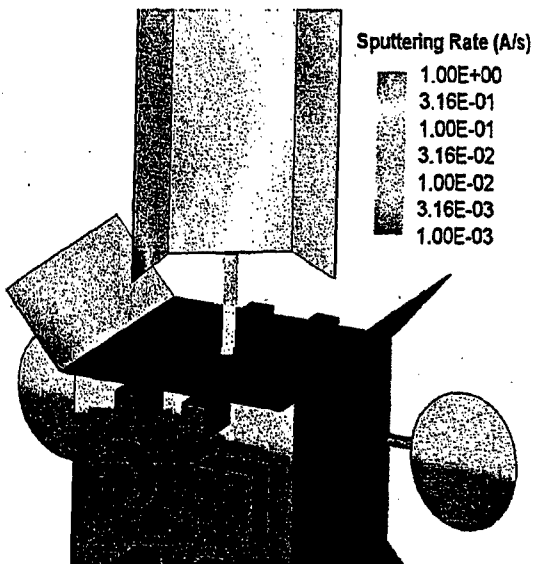


Fig. 7. Surface sputtering rate.

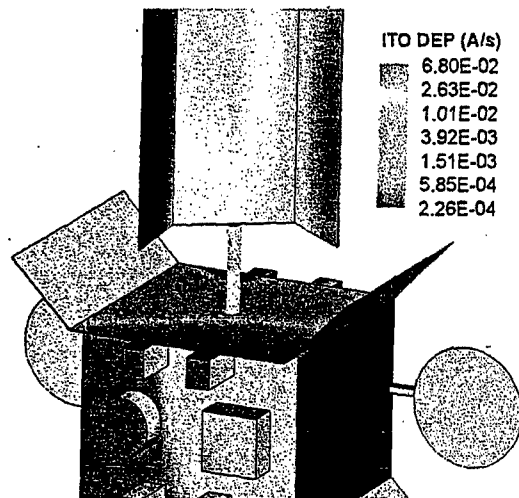


Fig. 8. Redeposition of ITO from the solar array cover glass to other spacecraft surfaces.

CASE 2 – Laboratory Vacuum Chamber with HET and Plume Diagnostic Instrumentation

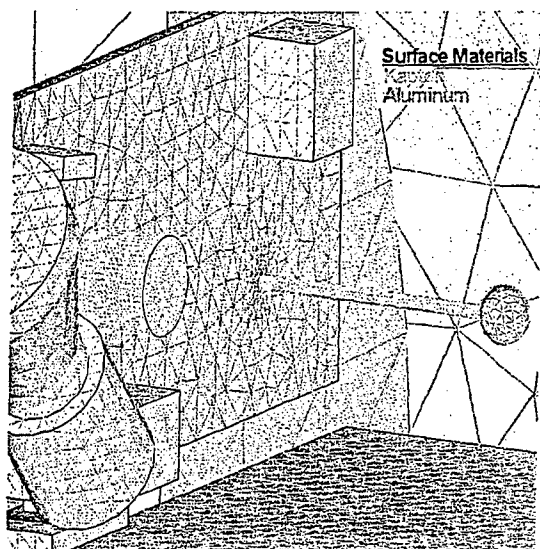


Fig. 9. Surface mesh of an HET inside a vacuum test facility with plasma measurement instruments.

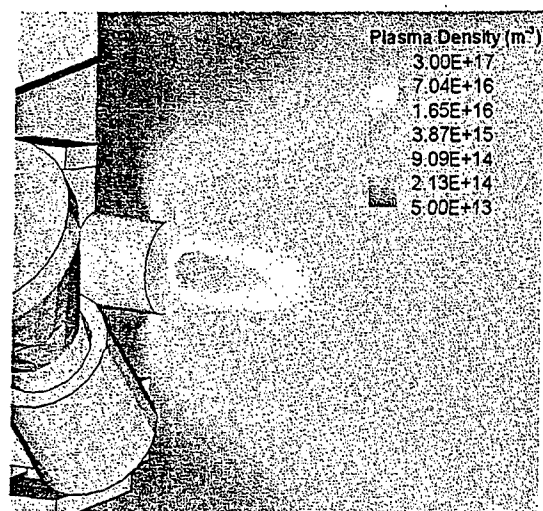


Fig. 10. Slice showing plasma density from a 200-Watt HET firing inside a vacuum test facility.

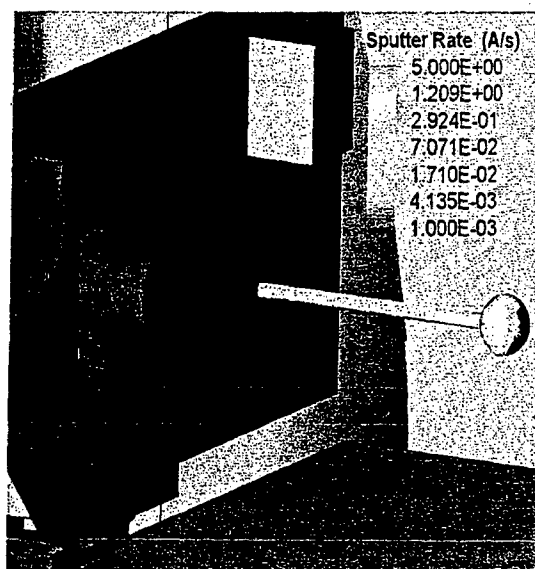


Fig. 11. Surface sputtering rate.

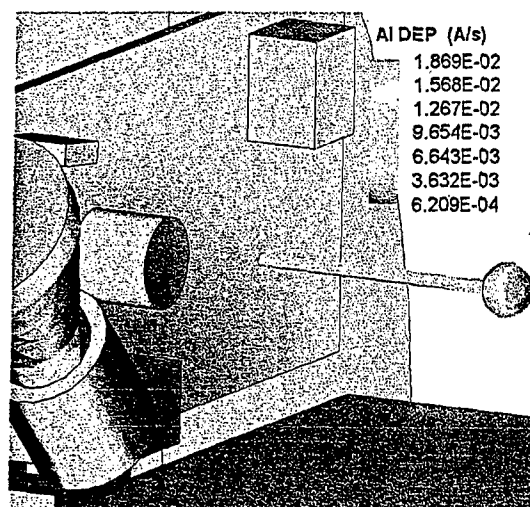


Fig. 12. Redeposition rate of aluminum from the chamber wall to instruments and surfaces on the HET test fixture.